STRAIN GRADIENT CRYSTAL PLASTICITY:
BRIDGING THE MICRO- AND MACRO- LENGTH SCALES

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ABSTRACT

A key part of multiscale material modeling is the bridging of the microscale dislocation dynamics and macroscale continuum plasticity theory. Currently dislocation dynamics simulations can handle a sample size typically on the order of microns or a few tens of microns. Therefore a continuum crystal theory which can accurately describe material deformation at micron scale is necessary for the successful bridging of the length scales. Conventional continuum theories assume that stress at a material point depends on state variables, primarily strain, at the same point only, and there are no length scales in the constitutive laws. The theories have long been proved to be adequate when the wave length of a deformation field is much larger than the dominant length scale of its micro-structure. However there have been accumulating experimental evidence showing that the conventional theories fail to perform adequately, at a typical size range of (a few tens of) microns. A strain gradient crystal plasticity theory has been proposed by Fleck and Hutchinson based on the notion of elevated hardening of a slip system due to geometrically necessary dislocations associated with slip gradient. In this talk, a possible venue will be discussed to obtain constitutive length scales and constitutive laws governing the non-local stress from homogenizing dislocation dynamics results.

As demonstration, a rate-dependent strain gradient crystal theory is applied to study (1) the deformation of a bicrystal and (2) the growth of a void in and the associated softening of a single crystal. A new finite element code, GRACY2D, has been developed to carry out the simulations. In the bicrystal, a narrow region around the grain boundary with non-uniform deformation is found and its width is well defined in terms of the constitutive length scale. The strain energy stored within the boundary layer therefore could be characterized as the change of the surface energy of the bimaterial due to deformation. Also predicted is the dependence of the overall yield stress of the bicrystal on the grain orientation mismatch and on the grain size. A full 3D calculation on a cluster of hundreds of grains has yet to be performed, but similar results are expected. The void growth in a single crystal is found to observe a strong void-size dependence. The relative elongation of a void with a radius on the same order of the constitutive length scale is found to be several times smaller than that of a much larger void whose behavior can also be modeled by a classical crystal theory. This suggests that at certain stress level only voids larger than a cut-off size can grow and coalescence, ie, small voids do not grow. The softening of the single crystal with a finite void concentration is also found to have a significant size effect.

To conclude, the strain gradient crystal plasticity theory bridges the microscale dislocation dynamics and macroscale continuum theories.